

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.96e-05 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.67e-01

Confidence level: 5.25e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Endrin aldehyde</div> <div>Measured: 6.30e-08</div> <div>Predicted: 1.07e-07</div>	<div>Image not found</div> <div>Dieldrin</div> <div>Measured: 5.80e-07</div> <div>Predicted: 3.60e-07</div>	<div>Image not found</div> <div>Endrin</div> <div>Measured: 5.80e-07</div> <div>Predicted: 3.60e-07</div>
<div>Image not found</div> <div>N-(1-Naphthyl)ethylenediamine</div> <div>Measured: 1.07e-02</div> <div>Predicted: 9.11e-02</div>	<div>Image not found</div> <div>4-Aminoacridine</div> <div>Measured: 6.00e-05</div> <div>Predicted: 1.96e-02</div>	<div>Image not found</div> <div>Napropamide</div> <div>Measured: 2.69e-04</div> <div>Predicted: 7.96e-04</div>